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FOR THE DEPARTMENT OF ENERGY

CRADA Final Report
for
CRADA Number 0695

Advanced Integration of Multi-scale Mechanics and Welding Process Simulation in Weld Integrity Assessment

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ABSTRACT

In this project, mathematical models that predict the microstructure in pipeline steel welds were to be developed. These models were to be integrated with thermal models that describe the time-temperature history in the weld as a function of location in order to derive the spatial variation of microstructure in the weld. The microstructure predictions were also to be combined with microstructure-hardness relations, based on the additivity principle, to determine the spatial variation of hardness in the weld. EMC2 also developed microstructural models based on empirical relationships. ORNL was to pursue the development of more fundamental, theoretically based models. ORNL applied a previously developed model for inclusion formation to predict the extent and nature of inclusions that form during weld cooling from the liquid. This inclusion model was directly integrated with computational thermodynamics capability. A convenient user interface was developed for both the inclusion model and the thermodynamic phase-stability calculations. The microstructure model was based on the simultaneous transformation theory analysis as applied to the transformation of austenite to various ferrite constituents during weld cooling. The model available on the Materials Algorithm Project web site was used. Extensive modification of this model was required to correct problems with compilation and calculations as a function of the computational platform (Unix, Linux, Windows, etc.) that was used. The user interface for the inclusion model and thermodynamic phase-stability calculations was delivered to EMC2 along with the modified and corrected microstructure model. Evaluation of the theoretically based model will be carried out and the predictions will be compared with experimental results as well as predictions based on the empirical models developed by EMC2.

INTRODUCTION AND OBJECTIVES

Models for predicting properties of low alloy steel welds that are used in pipeline applications have been under development for over three decades. The key objective of such models is to predict the extent of formation of low and high hardness regions. Low hardness regions represent softened zones and may indicate the presence of potentially weak zones that are prone to failure. High hardness zones represent regions with high fractions of bainite or martensite in the microstructure and these zones may have reduced ductility and increased susceptibility to hydrogen cracking.

Early models (1-3) predicted the conditions that produced a specific hardness value. These models identified the limits for welding conditions that were needed to avoid high hardness welds. They were based on empirical relationships derived from experimental results. The premise was that the weld conditions that were identified by these models provided a lower limit for heat input. In practice, if higher heat inputs were used then the welds would contain less bainite or martensite, they would be softer, and they would be less vulnerable to hydrogen cracking.

The next iteration of models (4-13), also based on empirical relationships, related the weld conditions and resultant thermal history to the maximum hardness present in the weld. Again, these models were developed to avoid excessive amounts of bainite and martensite. While these models provided more flexibility than the earlier models in that a maximum hardness was predicted, they were still limited in nature and their accuracy was limited as well.

The third iteration of models (14-19) was aimed at identifying the microstructure of welds as a function of thermal history. When combined with thermal models that determined the temperature versus time behavior in the weld as a function of both the location within the weld and the weld conditions, the spatial variation of microstructure could be identified. Using additive rules, the overall hardness was then predicted by summing the hardness contributions from each of the various microstructural constituents. These models were far more sophisticated than the first two generations of models. They used thermodynamic relations to identify critical transformation temperature limits and then applied kinetic relationships to determine the extent of formation of various austenite decomposition products (ferrite, pearlite, bainite and martensite) for a given thermal history. Most of these models used empirical relationships to identify the thermodynamic properties and the parameters in the kinetic equations.

The intent of this CRADA project was to develop new, improved models for microstructure and property prediction. Such models would be more robust, more accurate, and would be applicable to a wider range of alloy compositions. These models would also be integrated with other efforts in the overall project to relate microstructure and local properties to overall weld performance by utilizing advanced mechanics models.

APPROACH

For the successful prediction of weld microstructure and properties, the models must include four basic components. First, the model must accurately identify the thermal history as a function of location within the weld, based on the given welding conditions. Second, the model must identify the temperature ranges over which various phases are stable in order to identify the

phase transformations that may take place during the weld thermal cycle. Third, the model must be able to predict the microstructure evolution and the extent to which various phase constituents form, based on the calculated thermal history. Finally, the predicted microstructures must be related to the hardness.

The first part of the model, the prediction of weld thermal history as a function of weld conditions, was to be carried out by EMC2. Earlier models were to be improved, based on better and more refined mesh techniques that would allow for a finer spatial resolution in the thermal history predictions. A finer spatial resolution is critical since the thermal gradients in welds are quite severe and therefore the thermal exposure and resultant microstructure varies considerably with position.

The identification of phase stability as a function of composition and temperature is critical for the second part of the model. This component of the overall model was to be based on thermodynamic relationships. Early attempts at identifying the composition and temperature dependencies of phase stability were based on empirical relationships. In the last two decades new methods have been advanced which provide a more thorough and fundamental basis for thermodynamic predictions. Furthermore, the new approach, known as computational thermodynamics, is applicable to multicomponent systems and therefore is ideal for multicomponent commercial alloys. The flexibility of computational thermodynamics is also ideally suited for applications to a wider range of alloys and compositions, including new advanced alloys. ORNL was to integrate these advanced computational thermodynamics models into the overall model.

The third part of the overall model was to predict the microstructure based on the alloy composition and the weld thermal cycle. Two parallel approaches were to be used. EMC2 worked with the most advanced empirical models to integrate them into the overall model. On the other hand, ORNL investigated the potential application of more advanced, fundamental models. ORNL's task was to be divided into two tasks. The first task was to utilize new models for inclusion formation to predict the nature, size, and density of inclusions that form during weld solidification as a function of the thermal history and composition. Prediction of the inclusion population is important for two reasons. First, inclusions are known to have an important influence on the kinetics of the various austenite decomposition reactions. In fact, many recent alloy modifications have been made to promote the formation of specific inclusions in order to modify the final microstructural mix of ferrite, pearlite, bainite, and martensite. These modifications have been shown to lead to improved properties, especially toughness properties. Second, accurate prediction of inclusion populations also had the potential benefit of aiding the mechanics models that were being developed by others. The second task of the ORNL microstructure model development was the development of more fundamental and potentially more accurate microstructure models. These advanced models, in contrast to earlier models, were to be more basic in nature and not based on empirical kinetics relations.

The final component of the overall model was to relate the predicted microstructures to hardness. For both of the microstructure models (EMC2 and ORNL), the same approach was to be used. The rule of mixtures was to be applied to relate the hardness of individual microstructural components (ferrite, pearlite, bainite, and martensite) to the total hardness by using a weighted average of the hardness of each of the four microstructural constituents. Standard relationships between microstructure and hardness were to be used for both the ORNL and EMC2 models.

RESULTS

EMC2 Microstructural Model Development

While the development of a theoretically based microstructural model was pursued at ORNL (see below), EMC2 worked on the development of an alternative, empirically based microstructural model. The model was based on the work Kirkaldy and Venugopalan (14) but was to include the empirical parameters identified by Li et al. (17). It was to be integrated with an advanced thermal model developed by EMC2 that described the time-temperature evolution in the weld heat-affected zone. The model description and results of model calculations have been published (20,21).

Inclusion Model

Earlier work at ORNL (22) led to the development of a robust model for the prediction of inclusion formation during weld solidification. The model was based on advanced computational thermodynamics. The model predicted the types of inclusions that formed as a function of composition and temperature. As inclusions precipitated in the molten weld pool during cooling, the model accounted for the change in composition and the effect of this compositional change on the stability of inclusions. In this way, the sequential formation of inclusions was predicted and the model was validated with experimental results.

This inclusion model was implemented into the IGOR Pro software as part of the CRADA project. A user-friendly interface was created. Furthermore, the interface was integrated with computational thermodynamics software (ThermoCalc) so that the inclusion model could be applied in conjunction with state-of-the-art thermodynamics calculations. This interface was delivered to EMC2. Figure 1 shows the user interface. The thermal history is input as either a data file with temperature versus time or as an analytical expression for temperature as a function of time. Similarly, composition is entered. The calculation then determines the inclusion characteristics such as inclusion number density, inclusion volume fraction and overall inclusion composition (the actual inclusion population may consist of several oxide inclusion types that form during the overall weld cooling process). The results of a typical calculation are shown in Figure 2.

However, for several reasons the integration of the inclusion model interface into the overall model was never implemented. First, EMC2 never purchased the computational thermodynamics software that was integrated with the inclusion model. Instead they determined that the empirical thermodynamic routines were sufficiently accurate for their needs in some project applications. Second, EMC2 determined that the overall model was to be based on a Fortran code rather than the IGOR Pro software. Having a Fortran code rather than IGOR Pro software for the microstructure modeling was essential so that the microstructure predictions could be incorporated into the detailed weld numerical simulation software that uses the ABAQUS finite element code with user subroutines during weld simulation analyses. It was left up to EMC2 to attempt to translate the IGOR Pro code into Fortran for integration with other model components. EMC2 determined that this task was too tedious and the translation effort by EMC2 was dropped at the time it was needed to meet some project deadlines.

Application of Computational Thermodynamics

It was intended to use the commercial ThermoCalc code for carrying out the thermodynamic calculations as noted above. A user-friendly IGOR Pro interface was developed for using ThermoCalc. However, budget constraints prevented EMC2 from purchasing the computational thermodynamics code. Thus, this interface was not integrated into the overall model. Instead, ORNL provided support to EMC2 insofar as comparing calculations of phase stability and phase transformations using the ThermoCalc code with predictions based on the empirical models. It was concluded by EMC2 that the empirical predictions may be sufficiently accurate and it was decided that the empirical relationships would be used in the microstructural models developed by EMC2 as of the spring of 2007.

ORNL Microstructural Models

In contrast to the advanced empirically based microstructural models being implemented by EMC2, ORNL pursued the utilization and application of microstructural models based on fundamental phase-transformation theory. A model that considered the simultaneous transformation of austenite into various constituents during cooling was developed by Jones and Bhadeshia (23-25). This model has many advantages over the existing empirical models. It considered austenite decomposition at grain boundaries and at grain interiors and it considered various product forms of ferrite (allotriomorphic ferrite, acicular ferrite, etc.). The model accounted for changes in austenite composition as ferrite was formed. The model also allowed for simultaneous formation of various product forms as the temperature decreased, which is much more realistic than the earlier models in which one transformation reaction was shut down as another one was activated. Finally, the model also included the proven influence of inclusions on austenite decomposition. All of these features are neglected in the empirical models.

The simultaneous transformation model was available through the Internet and its application to this project was pursued. Two such codes were available, the original version ["Structure, v 2.0"(26)] and a revised version ["Structure2, v 3.0"(27)] that corrected some errors and also included Cu as a constituent. However, it was quickly determined that there were several errors in the downloaded versions of the software. Initially, these errors led to compilation errors. These problems were addressed but when they were overcome and the codes could be compiled on various platforms (PC, Linux, Unix, etc.), it was found that the codes yielded different results on different platforms for the same inputs. A major effort was undertaken to correct these errors. Eventually, the codes were modified so that they could be compiled and run on various platforms and the calculations on these various platforms yielded the same results. The modified and corrected versions of the code have been designated "Structure, v 2.0.1" and "Structure2, v 3.0.1". Unfortunately, this effort to correct the codes exhausted a major portion of the funding available at ORNL and further work on implementation of this code was severely curtailed.

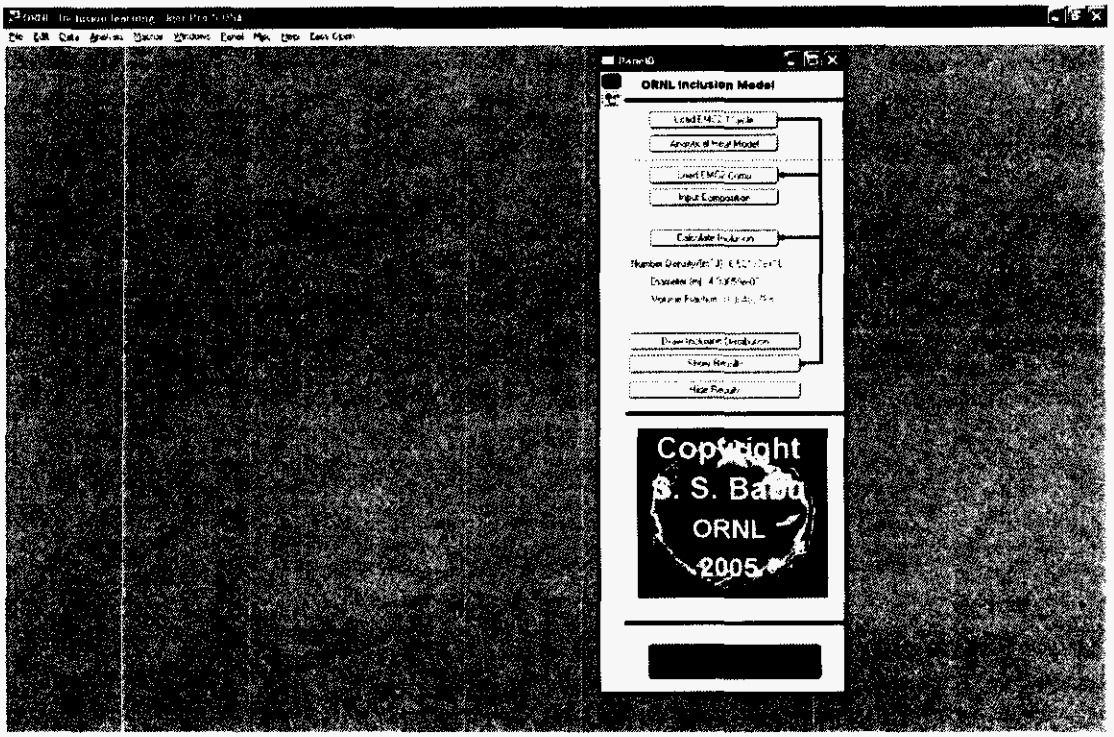

Fig. 1: Igor Pro interface for making inclusion calculations as a function of alloy content and thermal history.

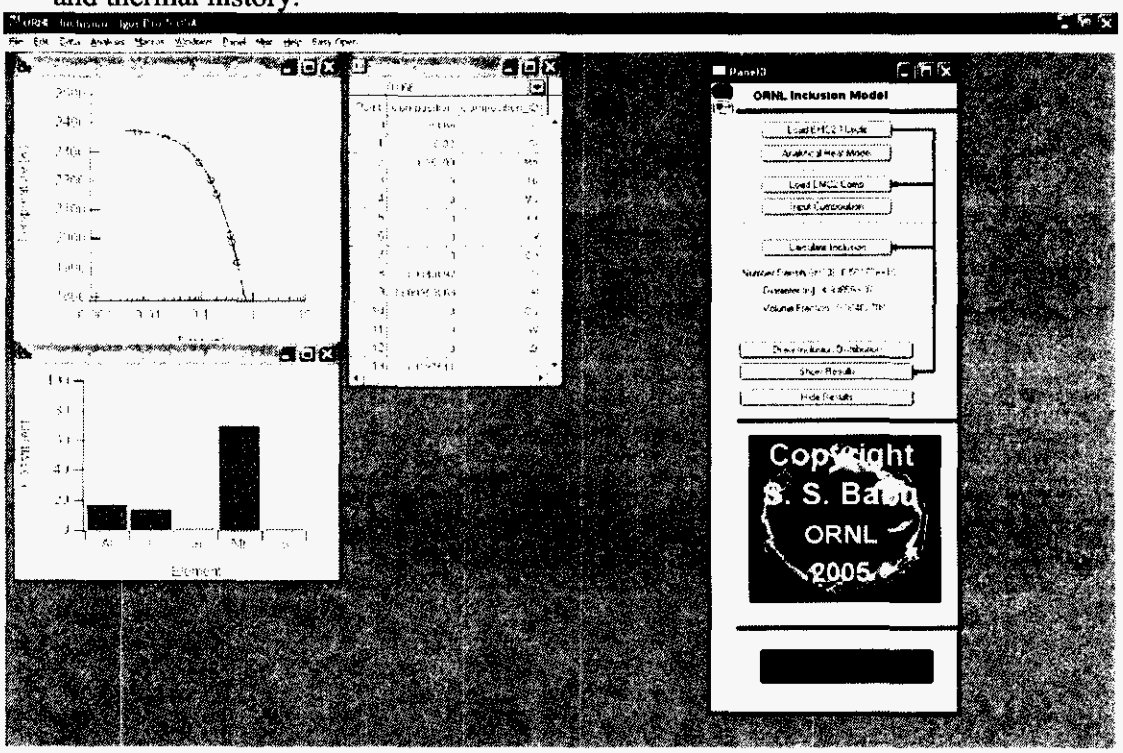

Fig. 2: Sample calculation results showing temperature-time history and overall inclusion composition in graphs and inclusion characteristics in window on the right.

Ultimately, it was decided that the advanced, fundamentally based code could not be utilized as the microstructural code in the overall project for some of the time critical deliverables. This decision was based on several points. First, while the codes predicted the decomposition of austenite into various forms of ferrite, and they also predicted the nature of this ferrite (grain boundary ferrite, inclusion-nucleated ferrite, matrix ferrite), they did not predict the formation of bainite or martensite. It would have been possible to estimate the proportion of these phases using other empirical routines, but this would have clearly been a compromise. Alternatively, the bainite and martensite could be lumped together, which might be acceptable if only looking for softening in a weld HAZ. Furthermore, the empirical codes and their parameters may not have been applicable since they were developed to describe the entire decomposition process and their application to just bainite and martensite formation may have been inaccurate. It is noteworthy that since the development and implementation of this code was temporarily abandoned, a revised code for somewhat similar alloys has become available (28) that includes bainite and martensite formation. It is expected that the same code corrections to Structure, v 2.0 and Structure2, v 3.0 that were identified in this program (yielding Structure, v 2.0.1 and Structure2, v 3.0.1, respectively) could be applied to the newer version of the software that includes bainite and martensite.

A second reason for temporarily abandoning the application of the Structure, v 2.0.1 and Structure2, v 3.0.1 codes was that after their modification and the correction of compiling errors and other errors, the results of the codes raised concerns. A parametric study of the effect of various input variables such as cooling rate, grain size, and inclusion content showed that reasonable results were found for the variation in structure as a function of cooling rate. However, changing the inclusion content seemed to have a minimal impact on the final microstructure mix, in contradiction to known experimental findings. Finally, the variation in microstructure with changing austenite grain size seemed to be opposite to the expected behavior. Some attempts were made to try to investigate the causes for these contrary results but funding ran out before the problems were resolved. It is believed that some basic modifications to the theoretical treatment may be needed. A listing of the corrected Structure and Structure2 codes is provided at the end of this report.

With the temporary abandonment of the application of the sophisticated Structure, v 2.0.1 and Structure2, v 3.0.1 codes, an alternative microstructural model was investigated. This model was based on the work of Kirkaldy and Venugopalan (14), as applied to welding by Watt et al. (15) and implemented into a Fortran code by Jaidi and Bhadeshia (29). This code was available through the Internet (29) and is similar to the EMC2 code in that both are empirically based, but the parameters in the codes are different. Once again, a few errors were found and corrected in this code. This code was delivered to EMC2 as an alternative to their microstructural code. The code did not have any grain growth routine included, which is an important deficiency since the austenite grain size is a critical variable in determining the final microstructure. However, implementation of such a routine should be relatively easy and it is likely that the same routine that is used in the EMC2 code could be used. An attempt was made to investigate the potential of modifying the code to account for some limited simultaneous transformation of austenite into various forms. It was found that inclusion of such a feature had a very strong impact on the final results. This same behavior is expected for the EMC2 code as well, since they are based on the same principles and their differences lie in the empirical coefficients used to identify the phase

transformation thermodynamics and kinetics. However, it was later concluded that such modification to include simultaneous transformation effects is inappropriate, even though they would be more representative of real behavior. This is because this model (and the EMC2 model) are empirical in nature and the parameters used in the empirical relationships are based on the premise that one transformation mode is shut off as another becomes activated. Thus, the identification of empirical parameters is contingent on this condition, regardless of whether the premise is real or not.

DISCUSSION

The primary goal of this project was to integrate microstructural models with thermal welding models and mechanics models. This goal was achieved by EMC2 using empirically based microstructure models. Experimental tests were performed by EMC2 to validate the model predictions and it was found that agreement between predictions and experiments were reasonable. However, limitations in accuracy were noted. The thermodynamic predictions based on empirical relationships were also found to be reasonable, based on comparisons with more detailed computational thermodynamic calculations made at ORNL.

There are several areas where further improvements are possible. With the use of empirically based thermodynamic predictions, one is limited to alloy compositions that lie within the range of alloys that were studied and used to develop the empirical parameters. Ultimately, it would be desirable to replace these empirical predictions with more flexible and robust computational thermodynamic routines. In this way, predictions for a broader range of alloy compositions could be made, including new modified alloy compositions.

The implementation of the fundamental, theoretically based, microstructure, prediction model would be desirable since this model would be more robust and could be used for a broader range of alloy compositions and even welding conditions. It would also properly account for the impact that the inclusions have on the microstructural development. However, the inconsistencies in the corrected model would need to be addressed. This might be a rather arduous task since it is possible that some of the theoretical descriptions of the transformations would need to be modified.

However, there are some on-going efforts in the DOE/PRCI project at EMC2 that are exploring the differences that exist between the predictions using the empirical Kirkaldy model and the Structure2, v 3.0.1 code for a large matrix of Gleeble specimens from an older X60 steel as well as from modern X70 and X100 steels. Predictions will also be compared to hardness profiles in actual welds made in an X70 and X100 steels. Dr. S. Babu of Ohio State University (Department of Industrial Welding and Systems Engineering and Department of Materials Science and Engineering) is involved in those efforts with the Structure2, v 3.0.1 code from this ORNL project. EMC2 staff will be conducting the Kirkaldy analyses in a round-robin fashion with Dr. Babu where the final hardness and microstructures in the matrix of Gleeble test results will be predicted with the same input parameters, same austenite grain growth model, and same hardness models, i.e., only the microstructure transformation models will be different. Finally, there are some features in the welds that neither the empirically based or theoretically based models take into account. None of the models deal with regions in the heat-affected-zone of the weld that are not reheated sufficiently high to re-austenitize the entire (local) microstructure.

Much work has been carried out over the last few decades on characterizing the austenitization kinetics but the models that have been developed based on that work deal only with re-austenitization. No current models consider both the transformation kinetics upon heating as well as the transformation kinetics upon cooling. For welds, both of these reactions are important and the ultimate model would include both types of reactions. However, inclusion of both of these reactions is far beyond the scope of this project.

CONCULSIONS

Improved microstructural models were developed and they will be integrated into the overall assessment and reliability models being pursued by EMC2. At present the empirical models are being incorporated into the broader code. However, additional work is underway at Ohio State University (not part of this CRADA) and EMC2 to evaluate the performance of both the empirical and theoretical models by comparing the predictions with recently generated experimental data.

BENEFITS TO THE FUNDING DOE OFFICE'S MISSION

Welding is one of the most important and widely used fabrication technologies in modern industry. Today in the United States, over 50% of the gross national products are associated with the production of welded products. The Industrial Materials for the Future (IMF) program of DOE OIT identifies welding and joining as one of the IMF multiple-industry research priorities. For many DOE OIT Industry of the Future (IOF) sectors, including petroleum, chemical, mining, metal casting, steel and forest product industries, the reliable performance of weld joints in various service environments can be the limiting factor for the safe operation and extended service life of equipment. This CRADA project is part of a larger program that aims to develop an advanced methodology that will be far more reliable and accurate than today's existing assessment techniques for evaluating the safety of welded structures used in the DOE Industry of the Future (IOF) and other industry sectors.

SUBJECT INVENTIONS

There are no inventions that have evolved from the completion of this project.

COMMERCIALIZATION POSSIBILITIES

While the specific microstructural modeling capability that has evolved from this CRADA project is not expected to be of commercial value, it will be integrated into a larger model that will assess the reliability and safety of pipeline welds. This larger integrated package is envisioned to be marketable and will be made available to appropriate industries on a commercial basis.

PLANS FOR FUTURE COLLABORATION

At the close of this project, there are no plans for further work on the microstructure models. However, this program did lead to a small Work-for-Others project to generate experimental data that will be used to validate the models.

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